

Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-
73771-63-8 | DTXSID50224153

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2210 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.89e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Acetylaminofluorene</div> <div>Measured: 1380</div> <div>Predicted: 1860</div>	<div>Image not found</div> <div>9-Anthracenecarboxylic acid</div> <div>Measured: 550</div> <div>Predicted: 1400</div>	<div>Image not found</div> <div>Anthraquinone</div> <div>Measured: 3720</div> <div>Predicted: 2300</div>
<div>Image not found</div> <div>9-Anthracenemethanol</div> <div>Measured: 4070</div> <div>Predicted: 5400</div>	<div>Image not found</div> <div>1-Amino-2-methylantraquinone</div> <div>Measured: 7940</div> <div>Predicted: 4960</div>	